

Self-Organization, Active Brownian Dynamics, and Biological Applications

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Abstract

After summarizing basic features of self-organization such as entropy export, feedbacks and nonlinear dynamics, we discuss several examples in biology. The main part of the paper is devoted to a model of active Brownian motion that allows a stochastic description of the active motion of biological entities based on energy consumption and conversion. This model is applied to the dynamics of swarms with external and interaction potentials. By means of analytical results, we can distinguish between translational, rotational and amoebic modes of swarm motion. We further investigate swarms of active Brownian particles interacting via chemical fields and demonstrate the application of this model to phenomena such as biological aggregation and trail formation in insects.

“Every theory, whether in the physical or biological or social sciences, distorts reality in that it oversimplifies. But if it is a good theory, what is omitted is outweighed by the beam of light and understanding thrown over the diverse facts.”

PAUL A. SAMUELSON

1 Introduction

About 1845, HERMANN VON HELMHOLTZ, the great pioneer in applications of physics to biological systems, developed the concept “*Physics of life*” (MARKL 1995) in companionship with his fellows EMIL DU BOIS-REYMOND, ERNST WILHELM VON BRÜCKE and CARL LUDWIG. Their statement,

that life is not in contradiction to physical laws, was later also elaborated by LUDWIG BOLTZMANN and others. But only in the 20th century, the investigations of ERWIN SCHRÖDINGER, MAX DELBRÜCK, LUDWIG VON BERTALANFFY, ILYA PRIGOGINE, MANFRED EIGEN, MIKHAIL VOLKENSTEIN and others led us to some understanding of the necessary conditions for the evolution of living systems (VOLKENSTEIN 1994). Their success was based on a specific theoretical approach to biological problems that also implied some reductionism. “Many biologists do not believe that ... biology can be given a theoretical foundation. Rather they insist in a holistic approach. ... Physicists, on the other hand, have not always appreciated that a theory of biology has to start from biological facts. They often thought that biology is just another field to which they could immediately apply their equations”. This quotation from EIGEN’s foreword to VOLKENSTEIN’S (1994) book indicates that the road to a fruitful collaboration between physicists and life scientists – the “*Helmholtz road*” – is full of obstacles. Nevertheless, we share the view that at the end of this road we are lead to some useful results, at least to some better understanding of biological facts. This shall also be demonstrated by the examples discussed in the following sections.

We start our considerations with some general remarks on self-organization and non-linear dynamics in biology. In particular, we summarize some basic physical principles that lead to the emergence of complex structures in biological systems, such as openness, irreversibility, entropy export and feedback processes. It is well known from the thermodynamics of irreversible processes that systems may exhibit a rich variety of complex behavior if there is a supercritical influx of free energy. This energy may be provided in different forms, i.e. matter (chemical components, resources), high temperature radiation, or signals. What kind of complex behavior is observed in a system, will of course not only depend on the influx of energy but also on the interaction of the entities that comprise the system. Among the prominent examples that can be observed in biological systems are processes of pattern formation and morphogenesis and different types of collective motion, such as swarming.

The main part of our paper is devoted to the modelling of active motion and coherent motion that in biological systems can be found on different scales, ranging from cells or simple microorganisms up to higher organisms, such as bird or fish. Our investigations are based on a model of active Brownian particles, i.e. particles with an internal energy depot that can be used for active movement. Considering further non-linear interactions between the particles, such as attractive forces or interactions via chemical fields, we are able to derive a rather general framework for the dynamics of swarms.

By means of both, computer simulations and analytical investigations, we demonstrate how the superposition of simple microscopic motions may result in a quite complex dynamics of the macroscopic system. In particular, we derive analytical expressions for the distribution functions that allow to distinguish between different modes of swarming behavior, such as translational, amoebic and rotational modes of collective motion. Eventually, we study the dynamics of swarms coupled to chemical fields and demonstrate the application of this model to phenomena such as biological

aggregation and trail formation in insects.

2 Self-Organization and Nonlinear Dynamics in Biology

2.1 General Aspects of Complexity

From our daily life experience we know how fragile and complex biological, ecological and social systems behave. What do we mean by the term “*complexity*” in a scientific context? According to our view complex systems are comprised of multiple components which interact in a nonlinear manner (cf. Fig. 1), thus the system behavior cannot be inferred from the behavior of the components. More specifically, these systems are characterized by (EBELING *et al.* 1998):

- structures with many components,
- dynamics with many modes,
- hierarchical level structures,
- couplings of many degrees of freedom,
- long-range spatial-temporal correlations.

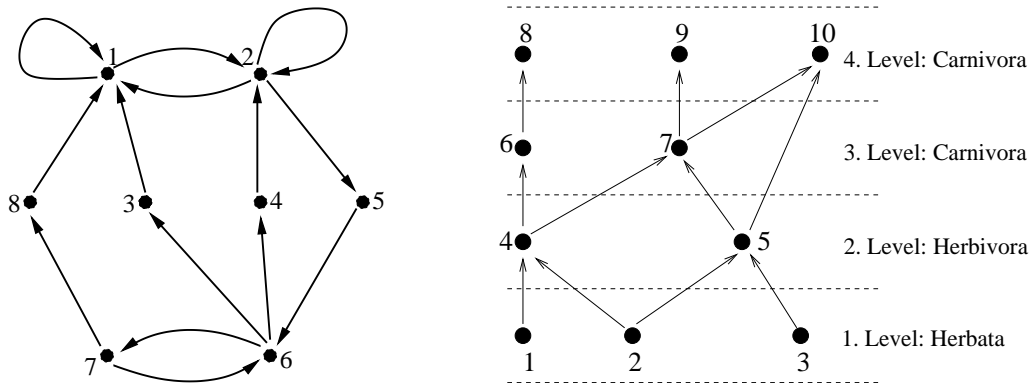


Figure 1: Two graphical representations of the interaction in complex systems: (left) a catalytical network consisting of 8 elements with 14 feedbacks, (right) a hierarchical ecological network.

As we have learned from nonlinear dynamics, complexity is not restricted to large hierarchical systems, also relatively simple dynamical models may show complicated behavior. Among the specific features of complex nonlinear processes, we mention:

- complicated trajectories and chaos,

- manifolds of spatial-temporal structures,
- the limited predictability of future behavior (positive Kolmogorov-Sinai entropy).

Further, we note that complexity may arise in dissipative as well as in conservative systems. In general complex systems in nature and society are of dissipative nature, i.e. they are based on energy “consumption” that allows self-organization processes. This, however, needs some physical requirements, such as:

- thermodynamic openness, i.e. the system exchanges energy, entropy and matter with the environment,
- that on average the system exports entropy, i.e. it imports energy of high value and exports energy of low value (cf. Fig. 2),
- that the system operates far from equilibrium, beyond a critical distance from the equilibrium state (cf. Fig. 3),
- that the causal relations in the system include (positive and negative) feedback and feedforward processes (cf. Fig. 1), i.e. the dynamics of the system is nonlinear.

For further details we refer to the literature (e.g. EBELING *et al.* 1990, EBELING and FEISTEL 1994).

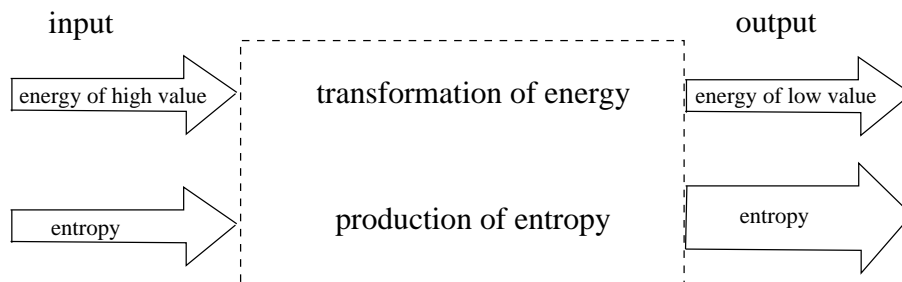


Figure 2: Transformation of energy and production of entropy in an open system: the export of entropy is a *conditio sine qua non* for self-organization.

2.2 Examples for physical models of biological systems

It is not intended here to give a complete overview of the vast applications of physical methods and tools to biological systems. Rather, we *pars pro toto* mention here only a few examples, where models based on the theory of self-organization and non-linear dynamics have contributed to our

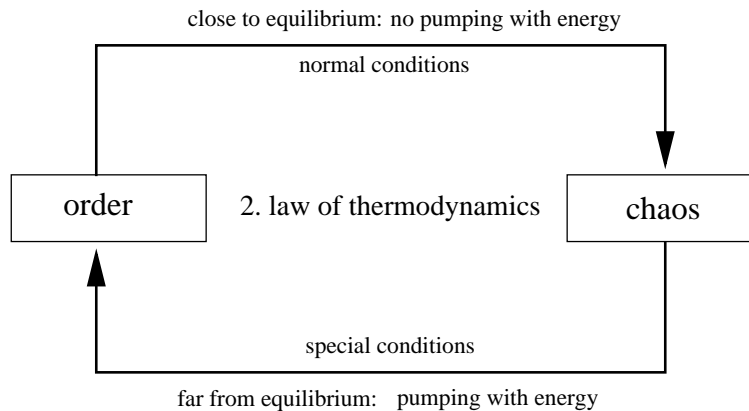


Figure 3: The 2nd law of thermodynamics allows different processes. Pumping with energy leads the system into states far from equilibrium which may be characterized by the emergence of ordered structures. The relaxation into the thermodynamic equilibrium, on the other hand, is accompanied by the disappearance of ordered structures.

understanding of biological phenomena (cf. also the other contributions in this volume and references therein):

- *Morphogenesis and biological pattern formation:* After the pioneering work on morphogenesis by TURING, MEINHARD, GIERER and others, today a well established theory on biological pattern formation exists that is based on the reaction-diffusion dynamics of several chemical components (morphogens). It has been successfully applied to a range of phenomena, such as patterning of animal coats or sea shells, pattern formation in bacterial colonies or slime molds, biological aggregation – but also to processes of regeneration and wound healing, organ differentiation, etc. (see e.g., the contribution by HOLSTEIN, this volume).
- *Biological rhythms and synchronization phenomena:* Given that the various functional units in biological systems act on different time and length scales, the emergence of synchronized behavior is by no means self-evident. Recent research in this direction has shown for instance how the brain activity is synchronized, or how cardiac cycles are triggered by excitation waves. As another example, the essential role of noise could be revealed in the case of stochastic resonance (see e.g. the contributions by BALASZI, BRAUN, KANTZ, MITTAG, MOSS, and SINGER, this volume)
- *Directed transport and molecular motors:* The ability of living cells to generate motion and forces, e.g. for mobility, contraction of muscles or material transport, could recently be understood within a physical description. For example, biological motor proteins which move along linear filaments can be described by stochastic models coupled to chemical reactions. So-called

ratchet models further explain the generation of directed motion on the microscopic level out of an undirected Brownian motion (see, e.g., the contribution by HÄNGGI, this volume)

- *Neural networks and associative memory*: The brain as one of the most complex systems known in biology, has also attracted the research activities of physicists since the pioneering work of HODGKIN, HUXLEY, HEBB, HOPFIELD and many others. It became clear that information is encoded not only in the response of the individual neural cells but also in the joint activity of a population of neurons. Based on these investigations, new techniques for information storage in associative memories or for pattern recognition, but also for brain stimulation have been developed. Artificial neural networks today also find a wide application in analyzing complex data sets (see e.g. the contributions by SINGER, by GRÜN and by TASS, this volume)

Despite a lot of successful investigations, we have to admit that many problems in the (physical) understanding of biological processes are still unsolved. Among the most important is the nature and the origin of biological information processing (EBELING and FEISTEL 1994, VOLKENSTEIN 1994).

In the following, we will restrict the discussion to a particular example, namely *active biological motion*, where we will show in more detail how a physical approach can be derived and on what reductions it is based.

3 Modeling active Brownian movement

3.1 Some historical remarks

Brownian motion denotes the erratic motion of a small, but larger than molecular, particle in a surrounding medium, e.g. a gas or a liquid. This erratic motion results from the random impacts between the atoms or molecules of the medium and the (Brownian) particle, which cause changes in the direction and the amount of its velocity, v .

The motion of the particle is named after the British botanist ROBERT BROWN (1773-1858), who in 1827 discovered the erratic motion of small pollen grains immersed in a liquid. He was inclined to explain his observation by so-called “active molecules”, and it is also reported that he wrote a letter to CHARLES DARWIN to ask him about his opinion on this subject.

BROWN was not the first who observed such a motion with a microscope. For example, already the Dutch ANTON VAN LEEUWENHOEK (1632-1723), who first discovered micro organisms with a simple microscope, knew about the typical erratic motion, however he considered it a feature of living entities. In 1785, the Dutch physician JAN INGENHOUSZ (1730-1799) also reported the

erratic motion of anorganic material dispersed in a liquid, i.e. powdered charcoal floating on alcohol surfaces, but this became not known to the non-Dutch speaking world.

The physical explanation of Brownian motion started about 1900 with the seminal works of ALBERT EINSTEIN (“On the theory of Brownian motion” 1905) and MARIAN SMOLUCHOWSKI (“On the kinetic theory of Brownian molecular motion and suspensions” 1906), but it should be noticed that already in 1900 LOUIS BACHELIER has derived a mathematical theory of this type of stochastic processes while investigating price changes at the stock market.

Brownian motion would be rather considered as *passive motion*, simply because the Brownian particle does not play an active part in this motion. It is an *undirected* motion, driven by thermal noise. Passive motion can also be directed, e.g. if it is driven by convection, currents or by external fields. Active motion, on the other hand relies on the supply of energy, i.e. it occurs under energy consumption and energy conversion and may also involve processes of energy storage. In order to add such a new element to the concept of Brownian motion, we need to investigate possible mechanisms of energy pumping.

The idea of energy supply was first introduced in the context of the theory of sound and music by HELMHOLTZ (“Die Lehre von den Tonempfindungen” 1870) and RAYLEIGH (“On maintained vibrations” 1883; “The theory of sound” 1877). The RAYLEIGH model of self-sustained oscillations is based on the assumption of a velocity-dependent friction coefficient (cf. Fig. 4), that can be negative for a certain range of velocity, i.e. instead of dissipating energy because of friction, energy can be pumped into the system. That means if a violin bow transfers energy to the string via friction *negative friction* occurs. Provided a supercritical influx of energy, a self-sustained periodic motion can be obtained, namely the violin string emits acoustic waves.

In the following we will show how the integration of the ideas about maintained vibrations and Brownian motion leads to a new model of *active movement*. This term will be used now for all kinds of motions in space and time which are driven by sources of free energy.

3.2 Brownian particles with energy supply

In this section, we introduce a simple stochastic model of active movement called “model of active Brownian particles” (SCHWEITZER *et al.* 1998, EBELING *et al.* 1999). Let us consider $i = 1, \dots, N$ active Brownian particles with mass m located at the positions \mathbf{r}_i and moving with the velocity \mathbf{v}_i . For the equation of motion we postulate:

$$m \frac{d\mathbf{v}_i}{dt} + \frac{\partial U}{\partial \mathbf{r}_i} = \mathbf{F}_i + \sqrt{2D} \boldsymbol{\xi}_i(t) \quad (1)$$

The last term denotes the stochastic force acting on the Brownian particle i with a strength D , the random function $\boldsymbol{\xi}_i(t)$ is assumed to be Gaussian white noise. U is the potential of external and

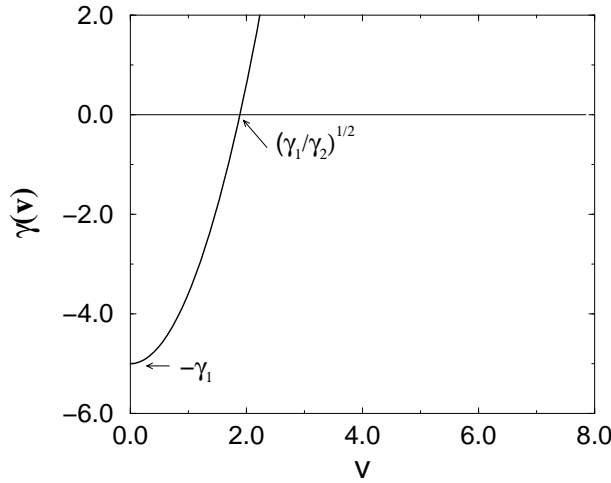


Figure 4: RAYLEIGH-type velocity-dependent friction coefficient $\gamma(v) = -\gamma_1 + \gamma_2 v^2$. For $\gamma(v) < 0$ “pumping” dominates, while for $\gamma(v) > 0$ “dissipation” dominates.

interaction forces and \mathbf{F}_i is the dissipative force acting on particle i . It can be specified as:

$$\mathbf{F}_i = -m\gamma\mathbf{v}_i + de_i\mathbf{v}_i \quad (2)$$

Here γ is the usual passive friction coefficient with the dimension of a frequency. We assume that the noise intensity D is related to the friction by an Einstein relation $D = m\gamma kT$, where k is the BOLTZMANN constant and T is the temperature. The second term $(d\mathbf{v}_i e_i)$ expresses an acceleration of the particle in the direction of \mathbf{v}_i (a forward thrust) which is based on the conversion of energy from a internal energy depot e_i of the particle. More specifically, we assume that the Brownian particle is able to take up energy with the rate q , which can be stored in an internal depot e_i . The internal energy can be converted into kinetic energy with a momentum dependent rate mdv_i^2 , which results in the acceleration in the direction of movement. The internal energy dissipates with the rate ce_i , The balance is then expressed by:

$$\frac{de_i}{dt} = q - ce_i - dv_i^2 e_i \quad (3)$$

If the internal energy depot relaxes fast compared to the motion of the particle, we find for eq. (2) in adiabatic approximation:

$$\mathbf{F}_i = -m\mathbf{v}_i g(v_i^2) = \mathbf{v}_i \left(\frac{dq}{c + dv_i^2} - m\gamma \right) \quad (4)$$

Here $g(v^2)$ denotes a velocity-dependent *friction function*. From now on we will use units corresponding to $m = 1$, i.e. $\mathbf{v} = \mathbf{p}$. Dependent on the parameter values, the dissipative force \mathbf{F}_i may

have one zero at $\mathbf{v} = 0$, or two more zeros with

$$\mathbf{v}_0^2 = \frac{q}{\gamma} - \frac{c}{d} \quad (5)$$

A nontrivial velocity $|v_0| > 0$ only exists if $qd > c\gamma$, i.e. if a supercritical supply of energy occurs. In this case, we also speak about “*active particles*”. For $0 < |v| < |v_0|$, i.e. in the range of small velocities the dissipative force \mathbf{F}_i is positive, i.e. the particle is provided with additional free energy. On the other hand, for $0 < |v_0| < |v|$, the dissipative force is negative. Hence, slow particles are accelerated, and fast particles are decelerated.

Assuming $v_0^2 > 0$ we consider now two limiting cases. Introducing the bifurcation parameter $\zeta = (dq/c\gamma) - 1$, we get for small values of the parameter ζ the well-known law of Rayleigh (cf. Fig. 4):

$$\mathbf{F} = \gamma\zeta \left(1 - \frac{v^2}{v_0^2}\right) \mathbf{v} \quad (6)$$

In the opposite case, i.e. for large values of ζ , we get the empirical law found by SCHIENBEIN and GRULER (1993) for the dynamics of cells:

$$\mathbf{F} = 2\gamma \left(1 - \frac{v_0}{v}\right) \mathbf{v} \quad (7)$$

This way, our expression for the dissipative force \mathbf{F}_i , eq. (4) is general enough to cover interesting limiting cases. We mention that in other models of driven motion (VISCEK *et al.* 1995) the velocity v_0 is postulated without further investigations.

3.3 Velocity distribution and mean squared displacement of free active motion

We are now interested in how known features of Brownian motion, such as the stationary velocity distribution or the mean squared displacement, change if we consider a supercritical energy take up ($qd > c\gamma$) of the Brownian particles. In order to find the velocity distribution explicitly we have to formulate and to solve the Fokker-Planck equation corresponding to Eq. (1). We restrict our consideration here to the two-dimensional space and $U = 0$, i.e. there are no external or interaction forces. Following standard procedures (KLIMONTOVICH 1995), we find from the Fokker-Planck equation the stationary solution for the velocity distribution (ERDMANN *et al.* 2000):

$$P^0(\mathbf{v}) = C \left(1 + \frac{d}{c} \mathbf{v}^2\right)^{\frac{q}{2D}} \exp\left(-\frac{\mathbf{v}^2}{2kT}\right) \quad (8)$$

Compared to the Maxwellian velocity distribution of “simple” Brownian particles, a new prefactor appears in Eq.(8) which results from the internal energy depot. For supercritical pumping, $qd > \gamma c$, we find a crater-like velocity distribution, which indicates strong deviations from the Maxwell distribution (cf. Fig. 5).

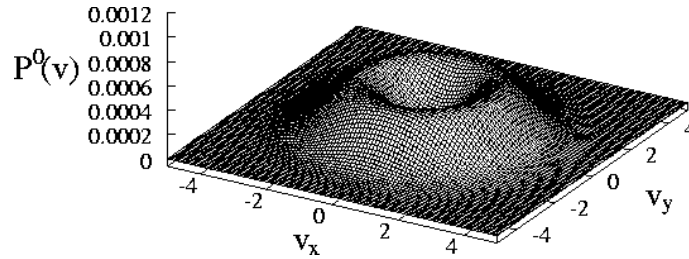


Figure 5: Stationary velocity distribution $P^0(\mathbf{v})$ for active Brownian particles in the case of super-critical energy supply (ERDMANN *et al.* 2000).

The distribution represented by Eq.(8) is an exact result for non-interacting particles. In the limit of zero noise, $D \rightarrow 0$, it obtains the form $\delta(v^2 - v_0^2)$. In this small noise limit, a result for the *mean square displacement* is also available (ERDMANN *et al.* 2000):

$$\langle (\mathbf{r}(t) - \mathbf{r}(0))^2 \rangle = \frac{2v_0^4}{D}t + \frac{v_0^6}{D^2} \left[\exp\left(-\frac{2Dt}{v_0^2}\right) - 1 \right] \quad (9)$$

From Eq.(9), we find the effective spatial diffusion coefficient of active Brownian particles as $D_r^{\text{eff}} = v_0^4/D$. This expression leads to rather large values for small D or large v_0 . The analytical expressions for the stationary velocity distribution and for the mean square displacement are in good agreement with computer simulations (SCHWEITZER *et al.* 2001) and with measurements on the active movements of granulocytes (SCHIENBEIN and GRULER 1993). We suggest to compare them also with the observations of the movement of *Daphnia* (see ERDMANN and MOSS, this volume).

4 Swarm dynamics with external and interaction potentials

4.1 Dynamics in external potentials

Let us now consider a swarm of active particles in a two-dimensional radially symmetric potential $U(r) = a(x_1^2 + x_2^2)$, that generates an attractive force towards the center, $r = 0$. As the snapshot of the spatial dispersion of the swarm shows Fig.6, we find the occurrence of two branches of the swarm, which after a sufficiently long time move on *two limit cycles*. One of these limit cycles refers to the left-handed, the other one to the right-handed direction of motion in the 2d-space.

The radius of the limit cycles can be calculated with the following considerations: Moving under stationary conditions, the particles have to comply with the additional requirement to balance between centrifugal and attracting forces, which leads to the condition $v^2/r = |U'(r)|$. For the harmonic potential this results in the stationary radius $r_0 = v_0/\omega_0$ where the frequency of rotations is given by $\omega_0^2 = a/m$ (ERDMANN *et al.* 2000).

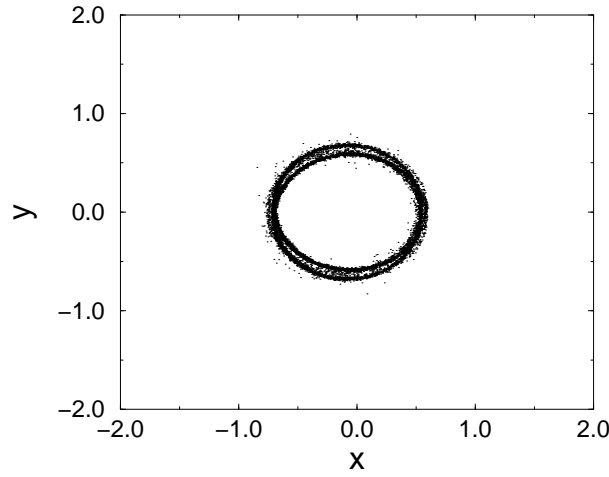


Figure 6: Spatial snapshot at $t = 99$ of a swarm of 10.000 active particles moving in a parabolic potential (SCHWEITZER *et al.* 2001).

For the motion on the limit cycle, an exact solution of the equations of motion reads in the deterministic limit:

$$\begin{aligned} x_1 &= r_0 \cos(\omega_0 t + \phi_0) & v_1 &= -r_0 \omega_0 \sin(\omega_0 t + \phi_0) \\ x_2 &= r_0 \sin(\omega_0 t + \phi_0) & v_2 &= r_0 \omega_0 \cos(\omega_0 t + \phi_0) \end{aligned} \quad (10)$$

Another exact solution is obtained by inversion. Any initial state converges to one of these attractor states. In the presence of fluctuations, the particles move in the neighbourhood of these two limit cycle orbits, which have circle-like projections and are located on two planes corresponding to the angular momenta $L = \pm v_0^2/\omega$. In this way, the probability is concentrated on two toroids in the 4-dimensional phase, the stationary distribution may be approximated by:

$$\begin{aligned} P^0(x_1, x_2, v_1, v_2) &= C \left[1 + \frac{d}{2c} (v^2 + \omega^2 r^2) \right]^{\frac{q}{2D}} \exp \left[-\frac{1}{2k_B T} (v^2 + \omega^2 r^2) \right] \times \\ &\times \left[1 + \frac{d}{2c} \frac{|L|}{r_0^2} \right]^{\frac{q}{2Dr_0^2}} \exp \left[-\frac{1}{2k_B T} \frac{L^2}{r_0^2} \right] \end{aligned} \quad (11)$$

Here the first factor represents a shell with given energy in the 4-dimensional phase space, while the second factor projects out two planes perpendicular to the two possible directions of the angular momentum, L . In this way two toroids in the 4-dimensional phase space are generated where the occupation density is concentrated.

4.2 Harmonic swarms

So far we have neglected any coupling within the swarm of active particles. If the swarm is not bound by an external potential as discussed above, the absence of interactions leads to the effect that the swarm eventually disperses in the course of time, whereas a “real” swarm would maintain its coherent motion. A common way to introduce correlations between the moving particles in physical swarm models is the coupling to a mean value. For example CZIROK *et al.* (1996) discuss the coupling of the particles’ individual *orientation* (i.e. direction of motion) to the mean orientation of the swarm. Other versions assume the coupling of the particles’ velocity to a *local average velocity*, which is calculated over a space interval around the particle (CZIROK *et al.* 1999).

Instead of an external potential $U(\mathbf{r})$, let us now assume an *interaction potential*. As the most simple case we may discuss the global coupling of the swarm to the *center of mass*. That means the particle’s position \mathbf{r}_i is related to the mean position of the swarm $\mathbf{R} = 1/N \sum \mathbf{r}_i$ via a potential $U(\mathbf{r}_i, \mathbf{R})$. For simplicity, we may assume a parabolic potential, i.e. the Hamiltonian for each particle reads now:

$$H_i = \frac{\mathbf{v}_i^2}{2} + \frac{a}{N} \sum_{j \neq i} (\mathbf{r}_i - \mathbf{r}_j)^2 \quad (12)$$

With respect to the harmonic interaction potential we call such a swarm a *harmonic* swarm (EBELING and SCHWEITZER 2001). The coupling to the center of mass corresponds to the assumption that there is now an attractive force between each two particles i and j which depends linearly on the distance between them. This can be used to control the dispersion of the swarm. A special case of nonlinear (exponential) interactions between particles on a chain has been analyzed in detail by EBELING *et al.* (2000).

Fig. 7 presents snapshots of a computer simulation of a harmonic swarm of 2.000 active particles.¹ Due to a supercritical take-up of energy, the particles are able to move actively, the interaction however prevents the swarm from simply dispersing in space. Thus, the collective motion of the swarm becomes rather complex, as a compromise between *spatial dispersion* (driven by the energy pumping) and *spatial concentration* (driven by the mutual interaction).

A closer inspection of the swarm dynamics (EBELING and SCHWEITZER 2001, SCHWEITZER *et al.* 2001) reveals that the system basically possesses two nontrivial dynamic modes. The first mode corresponds to a *flock-like swarm* moving coherently with given direction (translational mode). The second mode corresponds to a *rotating swarm* while the center of mass is at rest (rotational mode). Which of these modes is the target (attactor) of the collective motion depends both on the initial conditions and on the strength of noise.

Let us now characterize the two modes by means of the distribution functions. In the first mode, the particles move parallel to the velocity of the center of mass, V . Introducing the relative

¹A movie of these computer simulations – with the same parameters, but a different random seed – can be found at <http://ais.gmd.de/~frank/swarm-tb.html>

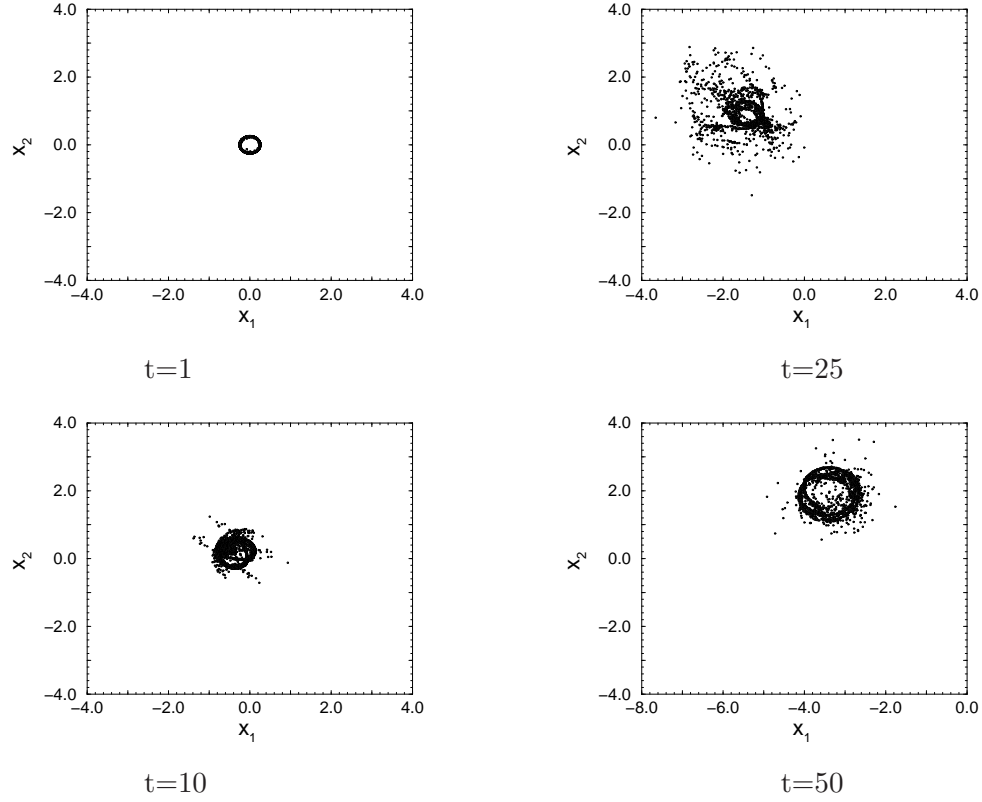


Figure 7: Snapshots (spatial coordinates) of a harmonic swarm of 2.000 active particles. t gives the different times. Initially, the particles were at rest and at the same spatial position. Note that the picture for $t = 50$ has a shifted x_1 -axis (EBELING and SCHWEITZER 2001).

velocity $\delta \mathbf{v}_i = \mathbf{v}_i - \mathbf{V}$, we get in first approximation the distribution:

$$P^0(\mathbf{r}_i, \mathbf{v}_i) = C \left[1 + \frac{d}{c} V^2 \right]^{\frac{q}{2D}} \exp \left[-\frac{V^2}{2kT} - \frac{a}{2kT} (\mathbf{r}_i - \mathbf{R})^2 \right] \times \exp \left[-\frac{1}{2\gamma kT} \left(g(V^2) (\delta \mathbf{v}_i)^2 + 2g'(V^2) (\mathbf{V} \cdot \delta \mathbf{v}_i)^2 \right) \right] \quad (13)$$

Here, $g(V^2)$ denotes the friction function introduced in Eq.(4), whereas $g'(V^2)$ is the first derivative of $g(V^2)$. According to Eq.(13), the square of the translational velocity V^2 is near to v_0^2 and the deviations fluctuate according to the Boltzmann distribution.

As we have shown by means of computer simulations (SCHWEITZER *et al.* 2001), the translational mode breaks down for small initial velocities $\mathbf{V}^2 \ll v_0^2$ (cf. also Fig. 7). In this case the velocities relative to the center of mass are amplified. On the other hand, the translational mode also becomes unstable if the dispersion of the relative velocities approaches the order of v_0^2 . In this way, the overall

picture is similar to the findings for the one-dimensional case (MIKHAILOV and ZANETTE 1999).

In the second stationary mode, where the center of mass is at rest $\mathbf{R} = \text{const.}$, $\mathbf{V} = 0$, the swarm is rotating around the center of mass, and we find in first approximation the distribution, Eq.(11) again, with H_i given by Eq.(12):

$$P^0(\mathbf{r}_i, \mathbf{v}_i) = C \left[1 + \frac{d}{2c} H_i \right]^{\frac{q}{2D}} \exp \left[-\frac{H_i}{2k_B T} \right] \times \left[1 + \frac{d}{2c} \frac{|L_i|}{r_0^2} \right]^{\frac{q}{2D r_0^2}} \exp \left[-\frac{1}{2k_B T} \frac{L_i^2}{r_0^2} \right] \quad (14)$$

The two possible branches of the rotating swarm correspond to the positive/negative angular momenta $L = m(x_1 v_2 - x_2 v_1)$.

There is still a third mode which is realized in the case of very strong noise, $k_B T \gg m v_0^2$. In this case the system does not feel the driving force anymore, hence it forms a Boltzmann distributed cluster with a stochastically moving center:

$$P^0(\mathbf{r}_i, \mathbf{v}_i) = C \exp \left[-\frac{H_i}{k_B T} \right] \quad (15)$$

In this way, we have – for a rather special model with linear attraction to the center – obtained a full stochastic description of three swarming modes. Despite our reductionistic approach, our findings agree also with the qualitative description of OKUBO and LEVIN (2001), who distinguish between three types of collective animal movement:

- *Rectilinear movement*: The animals as a whole tend to perform a rectilinear movement, thus forming a tight (cohesive) group.
- *Doughnut pattern*: When the forward thrust dominates the random force, a group of animals rotates around an empty center, forming the shape of a doughnut.
- *Amoebic movement*: When the random force dominates the forward thrust, the center of mass of animals hardly moves, though the shape of the group fluctuates around a circular pattern.

Hence, we conclude that even in the rather abstract description of physical swarm models, basic features of collective motion and swarm behavior can be recovered and, hopefully, also compared with biological observations of translating/rotating swarms of fish and birds.

5 Swarm dynamics in the presence of chemical fields

5.1 Models of biological aggregation

So far, we have assumed in our model that the linear attraction between any two members of the swarm is of physical nature. The results remain also valid if there is a *chemical* attraction directed

to the center of mass of the swarm. This is a reasonable assumption e.g. for the description of the dynamics of bacterial colonies (VICSEK 2001). Here, the chemotactic attraction might be responsible for the widely observed rotational movements of bacteria as *Bacillus circulans*, *Clostridium Tetani*, *Paenibacillus vortex*. If A is the chemotactic coefficient, the attraction of the active particles to the center is now given by a linear chemotactic force $\mathbf{F}_{ch} = -A\mathbf{r}$. In this case, the two characteristic quantities of our distribution functions derived above read as $\omega_0^2 = A/m$ and $r_0^2 = v_0^2 m/A$, and the dynamics discussed above remains the same.

A more elaborated investigation has to consider not only the response of the particles to the chemical signal, but also the generation of these chemicals by the particles, i.e. a non-linear feedback between particles and chemical. In order to describe the chemotactic response of the particles, we modify the Langevin Eq.(1), by replacing the potential U with a scalar field $h(\mathbf{r}, t)$ that describes the spatio-temporal concentration of the chemical. Assuming that the particles are attracted by higher concentration of the field, we find:

$$m \frac{d\mathbf{v}_i}{dt} + \left. \frac{\partial h(\mathbf{r}, t)}{\partial \mathbf{r}} \right|_{\mathbf{r}_i} = \mathbf{F}_i + \sqrt{2D} \boldsymbol{\xi}_i(t) \quad (16)$$

In a biological context, the chemical field can for example represent pheromones produced e.g. by ants or other insects in order to communicate with their mates, i.e. it can be envisioned as a communication medium that contains spatial information produced by the insects. The chemotactic response to the field is a basic feature of phenomena such as trail formation in ants (EDELSTEIN-KESHET *et al.* 1995, SCHWEITZER *et al.* 1997), it also plays an important role in the formation of biological patterns in bacteria *Escherichia coli* (BEN-JACOB *et al.* 1994) or slime molds (HÖFER 1999).

For the dynamics of the chemical field $h(\mathbf{r}, t)$, we assume the following reaction-diffusion equation:

$$\frac{\partial h(\mathbf{r}, t)}{\partial t} = \sum_{i=1}^N s \delta(\mathbf{r} - \mathbf{r}_i(t)) - k h(\mathbf{r}, t) + D_h \Delta_h h(\mathbf{r}, t) \quad (17)$$

It means that changes of the chemical concentration in space and time are governed by three processes: (i) production of chemical signals by the particles with a rate s at their current position, \mathbf{r}_i , (ii) decay of the chemical with a rate k , and (iii) diffusion (coefficient D_h).

The nonlinear feedback between the particles and the chemical field eventually results in the formation of aggregates, as the snapshots in Fig. 8 show. Biological aggregation based on chemotaxis is widely found in biological species, such as insect larvae (DENEUBOURG *et al.* 1990) or myxobacteria (STEVENS and SCHWEITZER 1997, DEUTSCH 1999) that gather guided by chemical signals originated by the individuals.

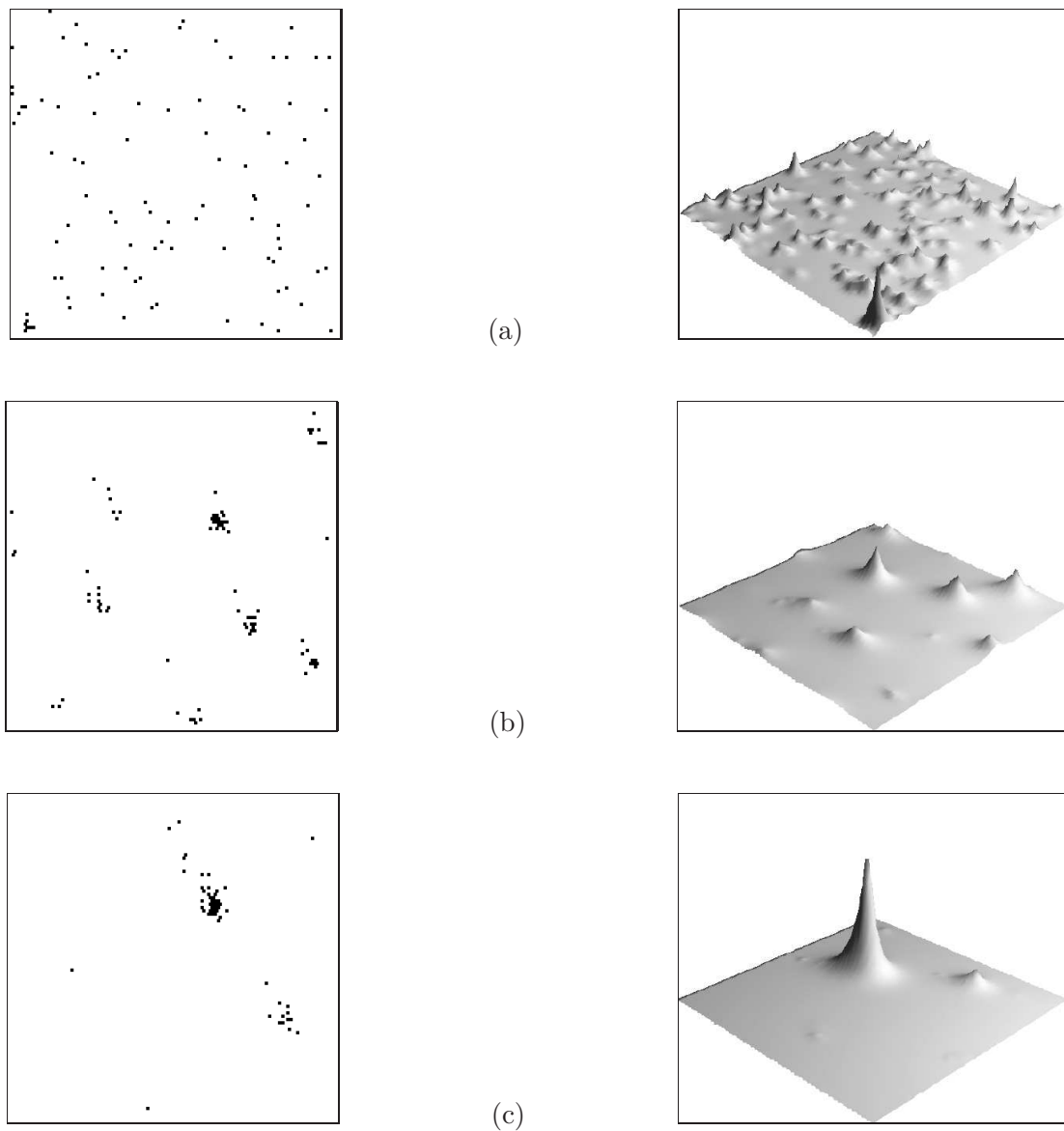


Figure 8: Snapshots of the positions of the active particles (left) and the distribution of the field (right) at different times: (a) $t = 100$, (b) $t = 5,000$, (c) $t = 50,000$. (SCHWEITZER and SCHIMANSKY-GEIER 1994)

5.2 Formation of Trails

A more complex dynamics of the particles can be obtained if instead of the simple chemoattraction described above different chemical fields and a more complex response of the particles to them are considered. So, let us eventually assume that the active particles have another internal degree of freedom θ_i , in addition to their internal energy depot e_i . The individual parameter θ_i may be used to describe different activities and responses to the field, i.e. the active particles then become *agents* with a more complex behavior (SCHWEITZER 2002).

For example, the production rate of the field, s , may now depend on the internal state $\theta_i \in \{-1, +1\}$, i.e. it becomes different for each particle i as follows:

$$s_i(\theta_i, t) = \frac{\theta_i}{2} \left[(1 + \theta_i) s_{+1}^0 \exp\{-\beta_{+1} (t - t_{n+}^i)\} - (1 - \theta_i) s_{-1}^0 \exp\{-\beta_{-1} (t - t_{n-}^i)\} \right] \quad (18)$$

Eq. (18) means that the active particle, dependent on its internal state θ_i may produce one of two different chemicals, $\{+1\}$ or $\{-1\}$, with a rate that exponentially decreases in the course of time. Consequently, we now have two different chemical field components that each are assumed to obey the following reaction equation (diffusion is not considered here):

$$\frac{\partial h_\theta(\mathbf{r}, t)}{\partial t} = -k h_\theta(\mathbf{r}, t) + \sum_{i=1}^N s_i(\theta_i, t) \delta_{\theta, \theta_i} \delta(\mathbf{r} - \mathbf{r}_i(t)) ; \quad \theta \in \{-1, +1\} \quad (19)$$

The effect of the two field components on each active particle may be described by an *effective field*, that also depends on the internal state θ_i of the agent, i.e. the gradient in eq. (16) shall be replaced by the gradient of the effective field (SCHWEITZER and TILCH 2002):

$$\frac{\partial h^e(\mathbf{r}, t)}{\partial \mathbf{r}} = \frac{\theta_i}{2} \left[(1 + \theta_i) \frac{\partial h_{-1}(\mathbf{r}, t)}{\partial \mathbf{r}} - (1 - \theta_i) \frac{\partial h_{+1}(\mathbf{r}, t)}{\partial \mathbf{r}} \right] \quad (20)$$

The nonlinear feedback between the active particles and the chemical field components can be summarized as follows: Particles with an internal state $\theta_i = +1$ contribute to the field by producing component $+1$, while they are affected by component -1 , and particles with an internal state $\theta_i = -1$ contribute to the field by producing component -1 and are affected by component $+1$.

Eventually, we assume that the particles can change their internal state from $\theta_i = -1$ to $+1$ and vice versa, dependent on environmental conditions or events. To be specific, we may consider that the active particles are initially concentrated in a “nest” ($\theta_i = +1$) and move out to search for “food”, distributed in different spatial locations. Once they found food, their initial state is changed to $\theta_i = -1$, which means that the successful particles begin to produce a different chemical (the “success pheromone”). This gives a new information to those particles that are not successful yet

to find the food sources, while the successful particle is guided back to the nest by the already existing chemical field component $\{+1\}$.

As the result of this non-linear feedback between the active particles communicating via two different chemical field components generated by them, we can observe the formation of directed trails between a nest and different food sources (cf. Fig. 9)

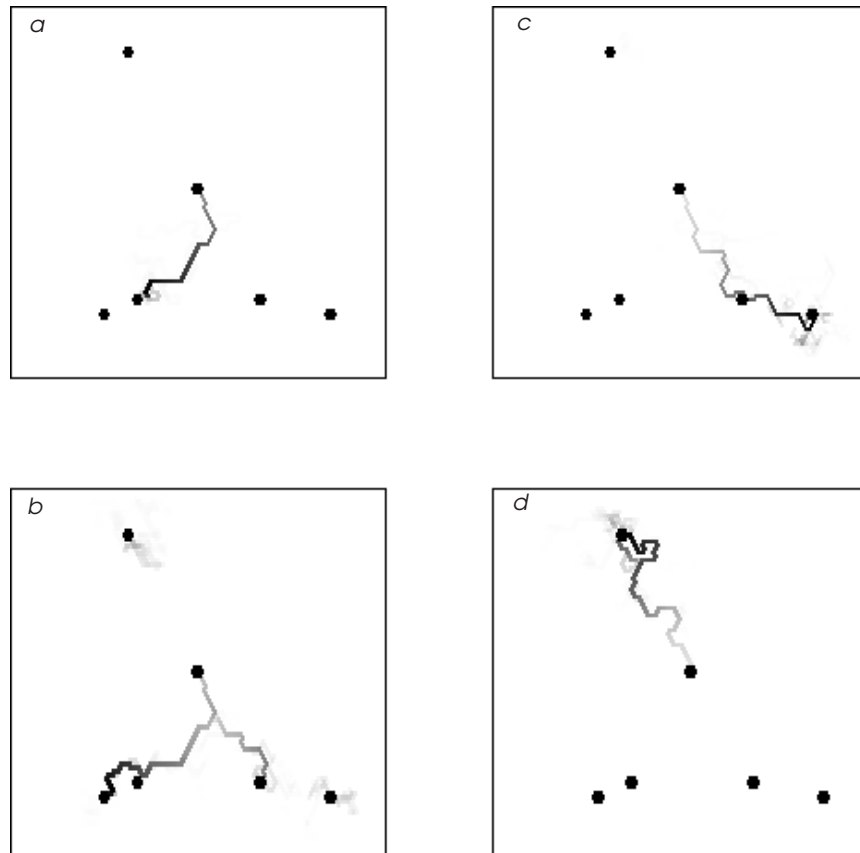


Figure 9: Formation of trails from a nest (middle) to five randomly placed food clusters, which are assumed to be exhausted after a number of visits. The distribution of chemical component $\{-1\}$ (see text) is shown after (a) 2000, (b) 4000, (c) 8500, and (d) 15000 simulation time steps, respectively (SCHWEITZER *et al.* 1997).

We note that, with respect to biology, there are different parameters which may influence trail following in addition to sensitivity, such as trail fidelity, traffic density, detection distance, endurance of the trail, navigation capabilities etc. (HAEFNER and CRIST 1994, EDELSTEIN-KESHET *et al.*, 1995). In contrast, our model considers only minimal assumptions for the trail formation. Here, the formation of trail patterns is solely based on simple *local* chemical communication between the

particles, with no additional capabilities of orientation or navigation. The spontaneous emergence of a collective trail system by means of the active particles can be described as a self-organizing process. It turns out from the computer simulations that, for different kinds of food sources, the model generates a distinctive trail system to exploit the food sources, and it performs a high flexibility in order to discover and to link new sources.

6 Conclusions

As the examples of the previous sections have shown, the approach of active Brownian particles provides a suitable framework to consider both the *energetic conditions* for active motion and the *interactions* between the particles – two ingredients essential for active and coherent movement in biological systems. The collective motion observed on the “macroscopic” level shows interesting analogies to swarming phenomena found in flocks of bird, schools of fish, but also in cells or insect societies.

With the established collective dynamics, we observe also the *emergence of new system properties* not readily predicted from the basic equations. This process was, in the beginning of this paper, described as *self-organization*, i.e. “the process by which individual subunits achieve, through their cooperative interactions, states characterized by new, emergent properties transcending the properties of their constitutive parts.” (BIEBRICHER *et al.* 1995). Whether or not these emergent properties occur, depends of course, not only on the properties of the system elements and their interactions, but – as we have pointed out in Sect. 2 – also on suitable external conditions, such as global boundary conditions, the in/outflux of resources (matter, energy, information).

For the prediction of the emergent properties from local interactions fundamental limitations exist which are discussed, e.g., in chaos theory. Moreover, stochastic fluctuations also give unlikely events a certain chance to occur, which in turn affects the real history of the system. This means, the properties of self-organizing systems cannot be determined by a hierarchy of conditions, the system creates its complexity in the course of evolution with respect to its global constraints. Considering, that also the boundary conditions may evolve and new degrees of freedom appear, co-evolutionary processes become important, and the evolution may occur on a qualitatively new level.

Within our physical approach to these phenomena, we are basically interested in the question *which extensions* to a known (physical) dynamics might bridge the gap towards a more complex (biological) dynamics. Such a stepping stone strategy is quite promising, as various applications for different biological problems have proven. Of course, many details of real biological phenomena have necessarily to be dropped, in order to focus on particular aspects. Let us quote in this context again from EIGEN’s foreword to the book of VOLKENSTEIN (1994): “The aim of theory is not to *describe* reality in every detail, but rather to *understand* the principles that shape reality.”

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